

Molecular Evolution in Collapsing Prestellar Cores

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ABSTRACT

We have investigated the evolution and distribution of molecules in collapsing prestellar cores via numerical chemical models, adopting the Larson-Penston solution and its delayed analogues to study collapse. Molecular abundances and distributions in a collapsing core are determined by the balance among the dynamical, chemical and adsorption time scales. When the central density n_{H} of a prestellar core with the Larson-Penston flow rises to $3 \times 10^6 \text{ cm}^{-3}$, the CCS and CO column densities are calculated to show central holes of radius 7000 AU and 4000 AU, respectively, while the column density of N_2H^+ is centrally peaked. These predictions are consistent with observations of L1544. If the dynamical time scale of the core is larger than that of the Larson-Penston solution owing to magnetic fields, rotation, or turbulence, the column densities of CO and CCS are smaller, and their holes are larger than in the Larson-Penston core with the same central gas density. On the other hand, N_2H^+ and NH_3 are more abundant in the more slowly collapsing core. Therefore, molecular distributions can probe the collapse time scale of prestellar cores. Deuterium fractionation has also been studied via numerical calculations. The deuterium fraction in molecules increases as a core evolves

and molecular depletion onto grains proceeds. When the central density of the core is $n_{\text{H}} = 3 \times 10^6 \text{ cm}^{-3}$, the ratio $\text{DCO}^+/\text{HCO}^+$ at the center is in the range 0.06-0.27, depending on the collapse time scale and adsorption energy; this range is in reasonable agreement with the observed value in L1544.

Subject headings: stars: formation — ISM: molecules — ISM: clouds — ISM: individual (L1544)

1. INTRODUCTION

Stars are formed in dense molecular cloud cores. Observations of cloud cores are very useful in the study of star formation; the structures and kinetics of star forming cores can be estimated via continuum and molecular line observations (Myers 1985; Benson & Myers 1989; Williams et al. 2000). Many cores with a young embedded protostar have been found and investigated following the infrared survey by IRAS (Beichman et al. 1986). These observations tell us about protostars and their envelopes *after* the formation of a protostar. In recent years, on the other hand, much effort has been done in the observation of cores in which the protostar is not yet formed, in order to understand the initial conditions and the earliest stages of star formation (André et al. 2000). Such dense molecular cores with no protostars are called starless or prestellar cores.

L1544 is one such prestellar core, and it is the most extensively studied so far. No sign of a protostar can be found toward L1544 by infrared and radio cm continuum observations. Detailed observations of mm dust continuum emission show that the gas density is high but almost constant, with the number density of hydrogen molecules $n(\text{H}_2) = 1.5 \times 10^6 \text{ cm}^{-3}$ inside a distance of 3000 AU from the emission peak (Ward-Thompson, Motte, & André 1999), also suggesting that the central star is not yet formed. In addition, molecular lines show a Doppler shift due to inward motion on the order of 0.1 km s^{-1} (Tafalla et al. 1998; Williams et al. 1999; Ohashi et al. 1999). Thus, L1544 must be in a very early stage of star formation.

Another interesting feature of L1544 is that there is a significant chemical differentiation within the core. Figure 1 shows that CCS is significantly depleted at the center of the core (Ohashi et al. 1999), while N_2H^+ is centrally peaked near the dust peak (Tafalla et al. 1998; Williams et al. 1999). The molecule C^{17}O shows a similar distribution to that of CCS, with a central hole of radius 6500 AU (Caselli et al. 1999). Such chemical differentiation has also been found in the prestellar cores L1498 (Kuiper, Langer & Velusamy 1996) and L1521F (Ohashi 2000 and references therein). In general, molecular abundances are essential in determining the structure of a core from line observations. Thus, it is important to investigate molecular distributions in collapsing cores with theoretical models.

In addition, the chemical differentiation within L1544 and similar objects can be a probe to investigate the infall time scale of the core, which is an important parameter for understanding the physics of star formation. Molecular distributions are determined by the balance between dynamical and chemical time scales. For example, molecular abundances should be constant throughout the core if the infall is much more rapid than the molecular evolution. If star formation is purely determined by gravity, the core should evolve roughly in a free-fall time scale. If other processes, such as magnetic field, rotation, or turbulence, are working against the collapse, the infall velocity is smaller, and the infall time scale should be much larger than the free-fall time scale.

Rawlings et al. (1992) have examined the evolution and distribution of molecular abundances in a collapsing core with the inside-out collapse solution of Shu (1977). This model corresponds to a protostellar envelope in which a central object exists, because the initial condition for inside-out collapse is a singularity at the center. Their results cannot be applied to prestellar cores such as L1544, in which the gas density is almost constant at the center. Bergin & Langer (1997) (See also Bergin 2000), on the other hand, have investigated molecular evolution in a prestellar core extensively. Two different dynamical models were examined: a dense cloud core contracting via ambipolar diffusion (Basu & Mouschovias 1994), and a phenomenological model where a static core is accreting material from a low density halo. They showed clearly that, in the collapsing core, sulphur-bearing molecules such as CCS deplete earlier than nitrogen-bearing molecules such as N_2H^+ , which is qualitatively consistent with the observation of L1544. They also showed that molecular evolution in each of their two collapse models shows a similar behavior as a function of time, and concluded that it is difficult to use chemistry to discriminate between different dynamical solutions. However, they investigated molecular evolution only with a single fluid element, and thus could not predict detailed distributions of molecular abundances, which should be compared with observations. Molecular distributions could be a probe to discriminate among dynamical solutions of the core.

This paper presents a theoretical model of the evolution of molecular *distributions* in *prestellar* cores, and constrains the collapse time scale of the core by comparison of the theoretical results with the observational data of L1544. As a standard model of the col-

lapsing core, we adopt the so-called Larson-Penston collapse, which is a self-similar solution for a purely dynamical isothermal collapse with spherical symmetry (Larson 1969; Penston 1969). The solution yields a density distribution in the core as a function of time in a semi-analytical form, which enables us to calculate molecular distributions in some evolutionary stages easily. In contrast to the inside-out collapse, the Larson-Penston solution corresponds to collapse prior to the formation of a protostar (Whitworth & Summers 1985), and thus is suitable for the study of prestellar cores. Numerical simulations show that the inner region of this solution is a good approximation for the “first collapse” phase of protostar formation (Masunaga et al. 1998; Masunaga & Inutsuka 2000).

The remainder of the paper is organized as follows. The dynamical model of the core and the model of molecular evolution are described in §2. §3 is concerned with calculated molecular distributions in a core undergoing Larson-Penston collapse, and the dependence of these molecular distributions on the collapse time scale, the sticking probability of gaseous molecules onto grain surfaces, the initial conditions, and adsorption energies for gas-phase species onto grains. In §4, the theoretical results are compared with the observations of L1544. Deuterium fractionation in the collapsing core is also discussed. Our summary is contained in §5.

2. Model

2.1. Model of Collapsing Core

We adopt the Larson-Penston solution (Larson 1969; Penston 1969) as our standard model for collapsing prestellar cores. The initial central density of the cloud is assumed to be $n_{\text{H}} = 2.0 \times 10^4 \text{ cm}^{-3}$, which is a representative value for molecular clouds. The temperature is assumed to be 10 K. Figure 2 shows the distribution of density n_{H} and infall velocity in the core at some evolutionary stages. The density distribution at $t = 1.89 \times 10^5 \text{ yr}$ is similar to that in L1544; in the central region the density is almost constant with $n_{\text{H}} \approx 3 \times 10^6 \text{ cm}^{-3}$, and in the outer region the density decreases as $n_{\text{H}} \propto R^{-2}$, in which R is the distance from the core center. The central densities at $t = 1.52 \times 10^5 \text{ yr}$ and $2.00 \times 10^5 \text{ yr}$, respectively, are smaller and larger than at $t = 1.89 \times 10^5 \text{ yr}$ by an order of magnitude. The density distribution ultimately approaches $n_{\text{H}} \propto R^{-2}$ throughout the core at $t = 2.06 \times 10^5 \text{ yr}$.

The numerical calculation is based on Lagrangian coordinates and follows molecular evolution in infalling fluid elements (or shells). Using the distribution of density and velocity at each time step (Figure 2), a temporal variation of the gas density in each fluid element is obtained. For instance, Figure 3 shows the density variation in several fluid elements as a function of time. The initial radius of the core is assumed to be $3.2 \times 10^4 \text{ AU}$, so that the core radius at $t = 1.89 \times 10^5 \text{ yr}$ is about the same as that of L1544 ($1.5 \times 10^4 \text{ AU}$).

2.2. Model of Molecular Evolution

The basic equations for molecular evolution are given by

$$\frac{dx(i)}{dt} = \sum_j \alpha_{ij} x(j) + \sum_{j,k} \beta_{ijk} x(j)x(k)n_{\text{H}}, \quad (1)$$

$$x(i) = n(i)/n_{\text{H}} \quad (2)$$

where $n(i)$ is the number density of species i , and α_{ij} and β_{ijk} are the rate coefficients. The first term on the right-hand side of equation (1) represents reactions with external particles such as ionization by cosmic rays. The second term represents two-body reactions in which species i are formed by the reactions of species j and k , or species i ($= j$) are destroyed by reactions with k .

For elemental abundances, we assume the so-called “low-metal” values (e.g. Lee et al. 1998; Aikawa et al. 1999). The initial molecular abundances are listed in Table 1. Gas phase species are in atomic or ionized form except for hydrogen, which is in molecular (H_2) form.

We have adopted the so-called “new standard model” network of chemical reactions for the gas-phase chemistry (Terzieva & Herbst 1998; Aikawa & Herbst 1999). The ionization rate by cosmic rays is assumed to be $\zeta = 1.3 \times 10^{-17} \text{ s}^{-1}$. In addition to reactions in the gas phase, the formation of H_2 molecules and the recombination of ions and electrons on grain surfaces are taken into account. The formation of ice mantles due to adsorption of gaseous molecules and the desorption of molecules from ice mantles are explicitly followed. The sticking probability S of neutral species when they collide with a grain is assumed to be 1.0 (Williams 1993). Uncertainty in the sticking probability and its effect on our results will be discussed later (§3.4). We adopt a grain radius of $1.0 \times 10^{-5} \text{ cm}$, which is considered to be a typical

value in interstellar clouds. Two kinds of desorptive mechanisms are included: thermal desorption, and non-thermal desorption via the impulsive heating of cosmic rays (Léger et al. 1985; Hasegawa & Herbst 1993). For simplicity and clarity, other chemical reactions on grain surfaces are not considered because the rates of grain surface reaction are still controversial (Caselli, Hasegawa, & Herbst 1998; Shalabiea, Caselli, & Herbst 1998).

In the outer region of the core, photodissociation dramatically reduces molecular abundances if the core is directly exposed to interstellar ultra-violet radiation. Considering that CCS is detected even in the outermost region of the core ($R \approx 15000$ AU), and that the core is embedded in a molecular cloud, $A_v = 3$ mag is assumed at the outer boundary of the core, so that the photodissociation does not much affect our model.

3. RESULTS

3.1. Molecular Evolution in an Infalling Fluid Element

Figure 4 shows the evolution of CO, CCS, N_2H^+ and some other species in an infalling fluid element. Molecules adsorbed onto grain surfaces are referred to as “ice” in the Figure and hereinafter. Gas-phase molecules decrease sharply in abundance at $t \sim 2 \times 10^5$ yr, mainly by adsorption onto grains. For the three gas-phase species we are mainly concerned with – CO, CCS, and N_2H^+ – the depletion time scales differ slightly. The abundance of the radical CCS decreases first, due both to adsorption and chemical reactions: CCS reacts with H_3O^+ or HCO^+ to produce HC_2S^+ , which is partially transformed to CS and then to CO. Even in a purely gas-phase model of molecular clouds with constant density ($n_H \sim 10^4$ cm $^{-3}$), CCS is well-known as an “early-time species”, the abundance of which has a peak at $t \sim 10^5$ yr, and decreases afterwards. The depletion of CO is mostly due to adsorption. The depletion time scale of N_2H^+ is larger than for the other species for the following three reasons. Firstly, N_2H^+ is not directly adsorbed onto grains. Since most grains are negatively charged at these densities (Umebayashi & Nakano 1980; Nakano & Umebayashi 1986), N_2H^+ recombines to produce N_2 , which returns to the gas phase and produces N_2H^+ again. Secondly, the nitrogen molecule N_2 , which is the precursor of N_2H^+ , is produced in the late stages of the gas-phase chem-

istry, and has a small binding energy on a grain surface. Thirdly, the main destroyers of N_2H^+ in the gas phase, CO and electrons, decrease in the later stages due to adsorption and the increased gas density. The N_2H^+ ion decreases in abundance eventually owing to the depletion of the main precursor, N_2 (Bergin & Langer 1997).

3.2. Spatial Distribution of Molecules

Radial distributions of molecules within the collapsing core at some fixed time steps are obtained by performing molecular evolution calculations similar to that described in the previous subsection for many fluid elements in the flow. Figure 5 shows such distributions in terms of absolute abundances (cm $^{-3}$).

At $t = 1.52 \times 10^5$ yr, most species in the figure are slightly more abundant in the inner region of the core, while CCS and C_3H_2 are less abundant in this region, where the gas density n_H is higher. If we plotted molecular abundances relative to hydrogen nuclei, instead of plotting absolute abundances, only SO_2 and N_2H^+ would be more abundant in the inner regions.

As the core evolves, the gas density in the central region becomes higher, which accelerates a further depletion of gaseous molecules. At $t = 1.89 \times 10^5$ yr, the spatial variation of the molecular density can be more pronounced than at $t = 1.52 \times 10^5$ yr. The molecules CCS and CO are depleted within a radius of several thousand AU, while N_2H^+ and NH_3 are still more abundant in the inner regions. At $t = 2.00 \times 10^5$ yr, even these nitrogen-containing molecules are slightly depleted at $R < 1000$ AU.

In order to compare our results with the observational data, molecular column densities in a spherical core are obtained by integrating along the line of sight. The effect of the integration is to average out the density dependence on R along the line of sight while preserving it in a direction perpendicular to the observer. Although the column density distribution is not as sharp as the distribution of abundances, it is unusual for the averaging to eliminate important radial dependences. Figure 6 shows distributions of column densities for assorted species at the three stages. Column density distributions for a larger number of species at $t = 1.89 \times 10^5$ yr are available in Table 2, designed for electronic presentation. CCS and C_3H_2 have a central hole at these three stages. On the other hand N_2H^+ and NH_3 are centrally peaked most of the time. At $t = 1.52 \times 10^5$ yr CO and HCO^+

are centrally peaked, and the CS column density is almost constant at the center, while at later stages these species have a central hole. Column densities of some species at the center do not monotonically change as the collapse proceeds; e.g., the central SO₂ column density increases from $t = 1.52 \times 10^5$ yr to 1.89×10^5 yr, but then decreases afterwards.

At $t = 1.89 \times 10^5$ yr, both the gas density and the molecular distributions are consistent with the observed characteristics of L1544. The dust continuum shows a gas density of $n_{\text{H}} \sim 3 \times 10^6 \text{ cm}^{-3}$ within the central region of radius about 3000 AU, while molecular observations show that CCS and CO have a central hole of radius about 7000 AU (Caselli et al. 1999; Ohashi et al. 1999), and N₂H⁺ has a peak near the dust peak (Tafalla et al. 1998; Williams et al. 1998). More quantitative comparisons are discussed in §4.1.

3.3. Dependence on Collapse Time Scale

If a core is partially supported by rotation (Matsumoto, Hanawa, & Nakamura 1997; Saigo & Hanawa 1998), magnetic fields (Basu & Mouschovias 1994) or turbulence, the collapse proceeds more slowly than in the Larson-Penston solution. This subsection shows how the molecular distribution depends on the collapse time scale in order to determine whether the dynamics of the collapse can be distinguished from molecular observations. It would be preferable if we could adopt an analytical or semi-analytical solution for the case of slow collapse due to magnetic fields or turbulence. Because no such solution is available, slow collapse models are constructed by artificially slowing down the Larson-Penston collapse by a constant factor; the inward velocity of the gas is divided by a factor f of 3 and 10.

Figure 7 shows molecular evolution in fluid elements for the Larson-Penston collapse and for a slower collapse with $f = 10$. Figure 8 shows results of the same evolution calculation, but as a function of the gas density in the fluid element at each moment. The molecular evolution in later stages ($t \gtrsim 10^5$ yr) can be seen more clearly in Figure 8. As discussed previously for the $f = 1$ case, the fractional abundances in Figure 7 (and Figure 8) are determined by a competition among chemical, adsorption and dynamical time scales. This competition is complex and is different for different species. For a molecule made relatively early and which is depleted mainly by adsorption onto grains at high densities, a slower collapse allows adsorption to proceed more efficiently. Car-

bon monoxide falls in this category, and the abundance of this species at $R = 3000$ AU (the inner radius considered) in Figure 7 is smaller in (b) than in (a). The abundance of CCS, an early-time species, at $R = 3000$ AU is also significantly smaller in (b) than (a). On the other hand, N₂H⁺ and NH₃ increase significantly at late stages in the slow collapse (b), when compared with (a). These so-called “late-time” species are produced slowly in the gas. In addition, depletion of the main destroying reactant — CO for N₂H⁺, and HCO⁺ for NH₃ — enhances their abundance (Bergin & Langer 1997). While SO₂ increases to $n(\text{SO}_2)/n_{\text{H}} \sim 10^{-10}$ within 2×10^5 yr in Figure 7 (a), it is almost constant ($\sim 10^{-12}$) at $t \sim 10^5$ yr, and increases to $\sim 10^{-10}$ at $t \sim 1 \times 10^6$ yr in the slow collapse (b), because its main formation path SO + O is more efficient at higher density. A decrease of HCO⁺, which is a principal destroyer of SO, also enhances the abundance of SO₂ (Bergin & Langer 1997). These formation reactions all become less efficient than adsorption in the final moment of the studied collapse, and the abundance of SO₂ at $R = 3000$ AU is significantly smaller in the slow collapse (b) than in the Larson-Penston case (a).

Figure 9 shows distributions of assorted absolute molecular abundances at the three evolutionary stages of the core for collapse slowed by factors of $f = 3$ and $f = 10$. The distribution of the total (hydrogen) density in the core is exactly the same as in Figure 5 for each panel (a-c), so these cores will be recognized as in the same physical evolutionary stage, if observed by dust emission. Comparison of Figures 9 and 5 shows that the molecular distribution clearly depends on the collapse model. The depletion of CO and CCS is more severe in the slow collapse cases, especially in the inner core (ex. $R \lesssim 5000$ AU at $t = f \times 1.89 \times 10^5$ yr). The radius of the region in which the absolute abundance of SO₂ has a peak value is larger in the slow collapse cases. The late-time species — NH₃, and N₂H⁺ — are more abundant in the slow collapse cases than in the Larson-Penston case (Figure 5), because of their slow formation in the gas phase and the depletion of some species which destroy them.

The column densities of assorted species at $t = f \times 1.89 \times 10^5$ yr for all collapse models ($f = 1, 3$, and 10) are shown in Figure 10. In spite of the fact that the physical structure of the core is exactly the same, the distributions of molecular column densities are significantly different from each other. The distributions of CO, CCS, CS, C₃H₂ and SO₂ show a

hole structure, and the width of the hole is larger (if not deeper) in the slower collapse cases. The column densities of CO, CCS, CS and C₃H₂ are smaller in the cases of slow collapse, while the column density of SO₂ does not change monotonically as a function of f . On the other hand, N₂H⁺ and NH₃ are centrally peaked in all three models, and their column density is larger for slower collapse. Clearly the molecular column densities and distributions in prestellar cores are strongly dependent on the collapse time scale, and can therefore probe the dynamics of collapsing cores, more specifically if collapse occurs in a free-fall time scale or more slowly owing to partial support by rotation, magnetic fields or turbulence.

3.4. Dependence on the Sticking Probability

The previous subsection showed that adsorption of gaseous molecules onto grains is a major contributor to molecular distributions in cores. The sticking probability S of molecules when they collide with a grain is, however, rather uncertain. Based on some experimental and theoretical work, S is estimated to be 0.1 – 1.0 at temperatures of ~ 10 K (Williams 1993). So far $S = 1.0$ has been assumed.

The dot-dashed lines in Figure 10 show the column densities of assorted molecules for the case with $S = 0.33$ and $f = 3$, while the solid lines show the case with Larson-Penston collapse and $S = 1.0$. Since the time scale of adsorption is inversely proportional to S , these two lines should be close, if the molecular distribution is determined simply by the balance between collapse and adsorption. The species CO and HCO⁺ show such behavior, which suggests that the collapse time scale cannot be estimated based only on CO and HCO⁺, unless the exact value of the sticking probability is known. On the other hand, the column densities of CCS and C₃H₂ are much smaller for $S = 0.33$ and $f = 3$ than for $S = 1.0$ and $f = 1$, because chemical reactions, as well as adsorption, are the main destruction mechanism of these “early-time species”, which suggests that they can be good probes of the collapse time scale and are relatively insensitive to S (compare the dotted and dot-dashed lines in Figure 10). The column densities of SO₂, N₂H⁺, and NH₃ are larger for $S = 0.33$ and $f = 3$ than for $S = 1$ and $f = 1$, because they are efficiently produced in the gas phase at late times. Thus, a low column density of CCS reinforced by high column densities of N₂H⁺ and NH₃ can be considered as a characteristic of slow collapse ($f > 1$), regardless of the uncertainty

in the sticking probability.

3.5. Dependence on the Initial Conditions

The initial conditions pose another source of uncertainty in the molecular evolution of a collapsing core. In the above calculations, the initial gas was assumed to consist of atoms and ions, with total gas density $n_{\text{H}} \sim 2 \times 10^4 \text{ cm}^{-3}$.

As an alternative, consider a Larson-Penston collapse starting from a gas density of $n_{\text{H}}(R = 0) = 2.0 \times 10^2 \text{ cm}^{-3}$, which is a representative value for diffuse clouds. The initial gas consists of atoms and ions except for hydrogen, which is in molecular form. In this model, the density distribution reaches the same values as that of the initial condition of the original model – $n(R = 0) = 2.0 \times 10^4 \text{ cm}^{-3}$ – after 1.85×10^6 yr. Then the subsequent evolution of the density distribution is the same as that of the original model with the time t of the calculation shifted by 1.85×10^6 yr; the central density of $n_{\text{H}} = 3.0 \times 10^6 \text{ cm}^{-3}$ is reached at $t = 2.04 \times 10^6$ yr, and the density distribution ultimately approaches $n_{\text{H}} \propto R^{-2}$ at $t = 2.06 \times 10^6$ yr. The dotted lines in Figure 11 show molecular column densities for this model at $t = 2.04 \times 10^6$ yr while the solid lines represent the original model at $t = 1.89 \times 10^5$ yr. Although the temporal gas density (n_{H}) distribution is the same for these two cores, the column densities of the assorted molecules are different. In the model with the lower initial density, CCS, CO, CS, and C₃H₂ are less abundant, and N₂H⁺, NH₃, and SO₂ are more abundant, because of the extended exposure to the chemistry, just as in the slow collapse model. But the absolute differences are not significant — only a factor of 2 or so — because the gas spent the initial phase (1.85×10^6 yr) at low density. More importantly, the radial profiles stay the same. Hence, our results are not significantly dependent on the choice of the initial density of the Larson-Penston collapse.

In a second alternative model, the physical evolution of the collapse is the same as that of the original model, but the gas consists mostly of molecules when the collapse starts. During the first $t = 3 \times 10^5$ yr, the cloud is supported by turbulence or magnetic fields, and the gas density stays constant with a typical molecular cloud value of $n_{\text{H}} = 2.0 \times 10^4 \text{ cm}^{-3}$. The duration of this pre-collapse phase is chosen because the molecular evolutionary model at this constant density reproduces the averaged abundances in molecular clouds, such as TMC-1 at around this time

very well (Millar, Farquhart & Willacy 1997; Terzieva & Herbst 1998). Then the support decays abruptly, for simplicity, and the gas collapses with a Larson-Penston flow. The dashed lines in Figure 11 show calculated molecular column densities vs R when the central density of the core reaches $n_{\text{H}} = 3.0 \times 10^6 \text{ cm}^{-3}$, i.e. $1.89 \times 10^5 \text{ yr}$ after the collapse starts. The deviations from the original model are more significant than in the first alternative model; CCS, CS, and C_3H_2 are decreased more than an order of magnitude, and SO_2 is increased by a factor of 5. Therefore, the duration of the pre-collapse phase can have an important effect in determining the molecular evolution in the collapsing core, if the gas density in the pre-collapse phase is as high as $n_{\text{H}} \sim 10^4 \text{ cm}^{-3}$. The deviation is less significant if the duration of the pre-collapse is shorter, or the density of the pre-collapse stage is lower.

3.6. Uncertainty in the Adsorption Energy

The desorption rate of molecules from the grain surface is another uncertainty in the theoretical model. Both thermal and non-thermal desorption rates are sensitively dependent on the adsorption (binding) energy of a molecule to the grain surface, but experimental data of adsorption energies are not yet available for many of the species included in our model. In addition, the binding energy is dependent on the nature of the grain surface, about which little is known, and which is likely to be time-dependent. For example, the binding energy of a CO molecule is 960 K on pure CO ice, and it is 1740 K on water ice (Sandford & Allamandola 1988; Sandford & Allamandola 1990). For simplicity and consistency with previous work, we have so far adopted adsorption energies for an SiO_2 surface, obtained for the most part theoretically by integrating the van der Waals interaction between a molecule and the surface (Allen & Robinson 1977; Hasegawa & Herbst 1993). This model is labeled as Model A hereinafter.

As an alternative (hereinafter Model B), some of the adsorption energies are replaced by the experimental data on pure ices. The modified values are listed in Table 3 together with the original values (Yamamoto, Nakagawa, & Fukui 1983; Sandford & Allamandola 1993; Aikawa et al. 1997). In Model B, the adsorption energies of non-polar molecules such as CO and N_2 are smaller, and the adsorption energies of polar molecules such as H_2O larger than in Model A. For species not listed in Table 3, the same val-

ues are adopted as in Model A (Hasegawa & Herbst 1993). Another alternative (Model C) corresponds to the “ H_2O ice mantle” of Bergin & Langer (1997), in which the original values are multiplied by a constant factor 1.47, which is a ratio of the binding energy of CO on H_2O ice to that on an SiO_2 surface.

Figure 12 shows assorted column densities at $t = 1.89 \times 10^5 \text{ yr}$ for the three models. The Larson-Penston collapse is assumed. The radial distribution of the column density of CCS is not much affected by the varied assumptions concerning the adsorption energy. On the other hand, the CO column density in Model B does not show a central hole, which is apparent in Model A, because net adsorption is too slow. If the ice mantle of the grain is as non-polar as pure CO ice, a slower collapse than the Larson-Penston collapse is preferable to account for the CO observations in L1544. The species N_2H^+ and NH_3 are not very sensitive to varying the adsorption energy. Although the adsorption energy of NH_3 is much larger in Model B than in Model A, NH_3 is still very abundant and centrally peaked because it is produced in the gas phase from N_2 at later stages. At $t = 2.00 \times 10^5 \text{ yr}$, however, N_2H^+ and NH_3 have a central hole of radius about 3000 AU and several hundred AU, respectively, in Model C. The species SO_2 is rather sensitive to the uncertainties of the adsorption energy; if the ice mantle is polar (Model C), its column density is significantly lower, and shows a central hole of radius 4000 AU, in contrast to the other two models. The ion HCO^+ , which is formed directly from CO, is more abundant in the central region in Model B than in Model A. In Model C, the column density of HCO^+ is higher than in Model A, in spite of the lower column density of CO, because the main destroyers of ions in the gas phase such as H_2O are less abundant in Model C. At $R \lesssim 5000 \text{ AU}$ the column density of C_3H_2 is higher in Model C than in other two models, because O atoms, which are a main destroyer of carbon-chain species, are more efficiently depleted from the gas phase. The depletion of O atoms in the inner regions has the same effect on the abundances of CS and CCS, but there are not significant changes in their column densities, which mainly derive from the outer regions.

4. DISCUSSION

4.1. Comparison with L1544

Our model results can be compared with observed molecular abundances in the prestellar core L1544, in an attempt to determine if the core is collapsing in a free-fall time scale (i.e. Larson-Penston collapse), or more slowly. The morphology of L1544 is in fact different from our spherical model; it has a flattened structure. But molecular column densities in L1544 can be compared with those obtained in our model, because L1544 is in an almost edge-on configuration (Ohashi et al. 1999), and because the free-fall time scale does not significantly depend on the elongation of the core.

Table 4 shows the characteristics of assorted molecular distributions in L1544 and theoretical models with a central gas density $n_{\text{H}} = 3 \times 10^6 \text{ cm}^{-3}$. In the theoretical models the initial condition is atomic, and Model A is assumed for the adsorption energies. In L1544, CO and CCS show a central hole of radius 6–8 thousand AU, and the peak column densities of CCS and CO are $4 \times 10^{13} \text{ cm}^{-2}$ and $2 \times 10^{18} \text{ cm}^{-2}$, respectively (Ohashi et al. 1999; Caselli et al. 1999; Caselli 2000, private communication). The exact radius of the hole is difficult to determine from the observational data because of the complex morphology and clumpiness of the core, especially for the CCS line. Among the four models listed in Table 4, the model with Larson-Penston collapse ($f=1$, $S=1.0$) is the most consistent with the observed distributions of CCS and CO, which means f should not be much larger than 1. In the Larson-Penston model the ratio of the CCS column density at the peak compared with the core center is about 1.4, which is also in reasonable agreement with the observed value. One objection against the Larson-Penston model might be that the infall velocity observed in L1544 ($\sim 0.1 \text{ km s}^{-1}$) is smaller than those in the outer region of the model (Figure 2). But this discrepancy is an effect of the outer boundary condition; Larson-Penston flow is a self-similar solution and does not take into account the fact that the flow velocity should be zero at a certain radius. In fact, numerical simulation of a collapsing core shows that the velocity in the outer region of the core is significantly smaller than the Larson-Penston solution, but that the dynamics of the core as a whole are similar to that of the Larson-Penston solution (Masunaga et al. 1998).

The column density of N_2H^+ is centrally peaked in L1544, and all models listed in Table 4 repro-

duce this distribution. However, the absolute value of the N_2H^+ column density obtained in our models is smaller than observed by a factor of 3–20. There are two possible explanations for this discrepancy. Since the model column density is smaller than observed in all four cases, the easiest solution would be to modify the reaction rate coefficient concerning the formation of N_2H^+ . The precursor molecule, N_2 , is formed by the reactions $\text{N} + \text{OH} \rightarrow \text{NO} + \text{H}$ and $\text{N} + \text{NO} \rightarrow \text{N}_2 + \text{O}$. Since the temperature dependence of the neutral-neutral reaction rates is not well known, these reactions may be a source of error in the theoretical model. But it is not probable that the error in the reaction rate coefficients causes the one-order-of-magnitude difference between the observation and the Larson-Penston model. Another explanation concerns the initial condition of the core formation. So far we have assumed that all the gases in the core start chemical evolution and collapse at the same time. But there is a possibility that the cloud is initially more inhomogeneous, and the prestellar core is formed by the coagulation of small clumps (Kuiper et al. 1996). The results shown in the previous section and Table 4 indicate that the discrepancy can be resolved if the gas parcels traced by N_2H^+ and CCS (and CO) have different “chemical ages”. While CCS cannot have experienced chemical evolution for much more than the free-fall time scale, the gas traced by N_2H^+ may have undergone chemical evolution for a longer time scale, because the N_2H^+ abundance increases as a function of time. Such a time difference would be naturally produced in an inhomogeneous model, with small clumps traced by CCS added to the central part of the core. Low UV attenuation in the small clumps would help to keep their chemical age young. A central part with more clumps would form a large core with higher density and attenuation by coagulation and collapse before the clumps in the outer region accreted onto it, and thus molecular evolution at the center would also proceed faster than in the outer region. It is also consistent with the clumpy structure of the L1544 core observed by the CCS line (Ohashi et al. 1999).

Readers may wonder if other uncertainties in the model, such as additional desorption mechanisms (e.g. photodesorption in the surface region) and temperature gradients in the core could affect the molecular distribution and resolve the discrepancy concerning CCS and N_2H^+ . For CCS, these uncertainties cannot change our result significantly, since the CCS

abundance decreases mainly because of chemical reactions in the gas phase. For N_2H^+ , very little precursor nitrogen resides on grain surfaces until very late times and the chemistry of formation is not particularly temperature dependent. So, this ion is also not likely to be affected strongly by these uncertainties.

Although we are confident of our qualitative conclusions, based on various parameter studies in §3, it is also true that more work needs to be done to constrain the uncertainties in chemical models, and to compare the model results with the observational data quantitatively. As one of such efforts, we are preparing another model calculation, in which full grain-surface reactions are included. More observations of different molecular species would be helpful, as well, in order to clarify the uncertainties in chemical models, the discrepancy concerning CCS and N_2H^+ , and the physical evolution of prestellar cores.

4.2. Deuterium Fractionation

Caselli et al. (1999) observed DCO^+ towards L1544, and found a high abundance ratio for $\text{DCO}^+/\text{HCO}^+$ of 0.12 ± 0.02 and 0.04 ± 0.09 at the position of the N_2H^+ emission peak for two separate velocity components, corresponding to background (blue) and foreground (red) components in the collapsing flow. In low temperature molecular clouds, ratios of deuterated to normal isotopes are much higher than the cosmic elemental abundance $\text{D}/\text{H} \sim 1.5 \times 10^{-5}$ because of the differences in zero-point energies between deuterated and non-deuterated species, and because of rapid isotopic exchange reactions (Millar, Bennet, & Herbst 1989). In addition, the deuterium isotopes are further enhanced once the heavy molecules start to be depleted (Brown & Millar 1989). For example, H_2D^+ is mainly formed by the reaction $\text{H}_3^+ + \text{HD} \rightarrow \text{H}_2\text{D}^+ + \text{H}_2$ and destroyed by the reactions with CO and with electrons. In most of the regions in our calculation, CO is the main reactant; although the rate coefficient of the reaction with electrons is about 3×10^2 times larger than that with CO, the electron abundance is much smaller than the CO abundance (see Figures 5 and 9). Thus the ratio $\text{H}_2\text{D}^+/\text{H}_3^+$ increases as the CO is depleted. This larger ratio leads to enhanced values for analogous ratios. In fact, the ratio $\text{DCO}^+/\text{HCO}^+ = 0.12 \pm 0.02$ in the blue-shifted component of L1544 is higher than the ratios $\text{DCO}^+/\text{HCO}^+ = 0.025\text{--}0.07$ in other “average” cloud cores in Taurus, which strengthens the argument that

the CO is depleted at the center of L1544 (Caselli et al. 1999). Since DCO^+ and HCO^+ are formed by the reaction of H_2D^+ and H_3^+ with CO, respectively, the ratio $\text{DCO}^+/\text{HCO}^+$ reflects the ratio $\text{H}_2\text{D}^+/\text{H}_3^+$. Deuterium chemistry has been included in our model to see whether or not the observed deuterium fraction can be reproduced and can yield some constraint on the model parameters. A detailed description of our deuterium chemistry network is found in Aikawa & Herbst (1999).

Figure 13 (a) shows the calculated column density ratio of DCO^+ to HCO^+ at three stages for our standard model with $f = 1$ and $S = 1.0$. The $\text{DCO}^+/\text{HCO}^+$ ratio increases as the core evolves, because of the depletion of gas-phase species. Figure 13 (b) compares our standard model with other cases. The ratio is higher in all cases with a heavier depletion of CO. Considering the rather wide range of the observed value in the “red” velocity component of L1544 ($\text{DCO}^+/\text{HCO}^+ = 0.04 \pm 0.09$), our models in Figure 13 (b) are consistent with the observation, except for the slow collapse with $f = 10$, which yields much too high a result. The value in the “blue” velocity component ($\text{DCO}^+/\text{HCO}^+ = 0.12 \pm 0.02$) is best reproduced in the case of Larson-Penston collapse with a high adsorption energy (Model C), although other models cannot be excluded because of the uncertainties in the observational data and in the chemical reaction rate coefficients.

5. SUMMARY

The evolution and distribution of molecules in collapsing prestellar cores have been investigated with the Larson-Penston collapse model.

The abundance for each molecule and its distribution in a collapsing core is determined by the balance between dynamical and chemical time scales (including adsorption). Because of differing chemical evolutionary patterns, molecular distributions differ for different species. In our standard model, when the central density of the core n_{H} rises to $3 \times 10^6 \text{ cm}^{-3}$ ($t = 1.89 \times 10^5 \text{ yr}$), the distributions of the CCS and CO column densities show a central hole of radius 7000 AU and 4000 AU, respectively, while the column density of N_2H^+ is centrally peaked, all of which is consistent with observations of the prestellar core L1544. If the collapse time scale is larger owing to rotation, magnetic fields or turbulence, the column densities of CO and CCS are much smaller, and their

central holes are larger than in the case of Larson-Penston collapse. The species N_2H^+ and NH_3 , on the other hand, are more abundant with slower collapse, and almost centrally peaked even if the collapse is slowed down by a factor of 10.

Several uncertainties in the theoretical model have been discussed, including the sticking probability onto grain surfaces, the initial physical and chemical conditions, and the adsorption energies of molecules on grain surfaces. Since the adsorption time scale is inversely proportional to the sticking probability, the abundance of CO, which is mainly determined by adsorption, is sensitively dependent on any assumption regarding the sticking probability. On the other hand, the depletion time scale of CCS is less affected by the sticking probability, because it is destroyed mainly by gas-phase chemistry. Those species that show little dependence on S are clearly better probes of the dynamics.

A change of the initial density in our model does not significantly affect the results; even if the Larson-Penston collapse starts with a density n_{H} of $2 \times 10^2 \text{ cm}^{-3}$, appropriate for diffuse clouds, molecular column densities are different from our standard model by at most a factor of 2 and the radial distributions are similar when the central density of the collapsing core reaches a certain value. The results are affected if we include a pre-collapse stage lasting $3 \times 10^5 \text{ yr}$ with gas density $n_{\text{H}} = 2 \times 10^4 \text{ cm}^{-3}$. Here the CCS column density is smaller than the standard case by more than an order of magnitude when the central density of the core reaches $3 \times 10^6 \text{ cm}^{-3}$, while the late-time species, especially SO_2 and N_2H^+ , are more abundant. The difference from our standard model is less significant if the pre-collapse stage is shorter or the gas density is smaller.

The dependence of our results on the uncertainty in grain adsorption energy is mixed. The CCS, N_2H^+ , and NH_3 column densities are not significantly affected by this uncertainty. The case of CO is another story; if the grain surface is covered by non-polar ice, and the adsorption energy of CO is as low as that for pure CO ice, its column density does not show the apparent hole structure at $t = 1.89 \times 10^5 \text{ yr}$ in the Larson-Penston collapse, which is inconsistent with the observation of L1544.

Comparison of our results with the observed molecular column densities in L1544 shows that our standard model with Larson-Penston collapse ($S = 1.0$, $f = 1$) is more consistent with the distributions (column

density and hole radius) of CCS and CO than slower collapse models. Since the column density of CCS is not much affected by the uncertainty in sticking probability and adsorption energies, and is sensitively dependent on the slowing down factor f , it gives a more strict constraint on the collapse time scale of L1544 than does CO. Moreover, the calculated distributions of N_2H^+ in our models are all centrally peaked, which is consistent with observation, regardless of the collapse time scale. However, the absolute value of the N_2H^+ column density is smaller than observed in all of our models, and the agreement is the worst in the Larson-Penston case. The most probable explanation is an inhomogeneous initial condition of the core (Kuiper et al. 1996), in which small clumps traced by CCS coagulate with the central core with high density and UV attenuation traced by N_2H^+ .

The deuterium fraction in molecules increases as the core evolves and heavy molecules reside on dust grains rather than in the gas. When the central density of the core is $n_{\text{H}} = 3 \times 10^6 \text{ cm}^{-3}$, the $\text{DCO}^+/\text{HCO}^+$ ratio at the center is calculated to lie in the range of 0.06-0.27, depending on the collapse model and the adsorption energies, which is in reasonable agreement with the observed range in L1544.

In conclusion, we have shown that the distributions of molecular column densities are probes of the collapse time scale of prestellar cores, if compared with theoretical models quantitatively. On the theoretical side, further consideration of uncertainties in the model, such as the homogeneity of the initial conditions and grain-surface processes, is desirable. On the observational side, mapping of other molecular lines of both early-time species (e. g. carbon chains) and late-time species (e. g. NH_3 and SO_2) would be helpful in order to reveal the evolution of the prestellar core L1544, and reduce the uncertainties in the chemical models. Statistical observations of molecular distributions in a large number of prestellar cores are desirable in order to reach more general conclusions on the physical and chemical evolution of these cores.

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Fig. 1.— Total intensity map of N_2H^+ (contours, Tafalla et al. 1998) and CCS (gray scale, Ohashi et al. 1999) in L1544. The cross shows the peak of dust continuum emission.

Fig. 2.— Distribution of (a) density and (b) velocity in a collapsing core with the Larson-Penston solution. The dotted lines show the initial condition ($t = 0$) of the core. The age of the core for other lines is 1.52×10^5 yr (*dashed lines*), 1.89×10^5 yr (*solid lines*) and 2.00×10^5 yr (*dot-dashed lines*).

Fig. 3.— Temporal variation of density n_{H} in infalling fluid elements that migrate from 8.2×10^3 AU to 1.0×10^3 AU (*solid line*), 1.9×10^4 AU to 5.0×10^3 AU (*dotted line*), 2.6×10^4 AU to 9.0×10^3 AU (*dashed line*), and 3.1×10^4 AU to 1.3×10^4 AU (*dot-dashed line*) in 2.00×10^5 yr.

Fig. 4.— Evolution of molecular abundances in a fluid element that migrates from 8.2×10^3 AU to 1.0×10^3 AU in 2.00×10^5 yr, while the gas density (n_{H}) varies from 1.7×10^4 cm^{-3} to 5.8×10^6 cm^{-3} .

Fig. 5.— Distribution of molecular abundances at (a) $t = 1.52 \times 10^5$ yr, (b) $t = 1.89 \times 10^5$ yr, and (c) $t = 2.00 \times 10^5$ yr in a core with the Larson-Penston flow. The central density (n_{H}) of the core is 3×10^5 cm^{-3} (a), 3×10^6 cm^{-3} (b), and 3×10^7 cm^{-3} (c).

Fig. 6.— Molecular column densities vs distance from the center in a Larson-Penston core at $t = 1.52 \times 10^5$ yr (*dotted lines*), 1.89×10^5 yr (*solid lines*), and 2.00×10^5 yr (*dashed lines*).

Fig. 7.— Molecular evolution in a fluid element that migrates from 1.5×10^4 AU to 3.0×10^3 AU in (a) 2.00×10^5 yr, and (b) 2.00×10^6 yr. The Larson-Penston collapse is assumed for (a), while the collapse is slowed down by a factor f of 10 in (b).

Fig. 8.— Molecular evolution in a fluid element as a function of gas density. Thick solid lines show the time, with labels on the right hand side of the figure, as a function of density. Other details are the same as in Figure 7.

Fig. 9.— Molecular distributions in cores with slow collapse. The collapse time scale is larger by a factor of $f = 3$ (*left panel*) and 10 (*right panel*) compared with the Larson-Penston solution. The age of the core is (a) $t = f \times 1.52 \times 10^5$ yr, (b) $f \times 1.89 \times 10^5$ yr, and (c) $f \times 2.00 \times 10^5$ yr.

Fig. 10.— Column densities of assorted species at $t = f \times 1.89 \times 10^5$ yr plotted vs R . The solid lines are for the Larson-Penston collapse ($f = 1$), the dotted lines are for slow collapse with $f = 3$, and the dashed lines are for $f = 10$. The sticking probability is assumed to be $S = 1.0$ for these lines. The dot-dashed lines are for the case of $f = 3$, but with lower sticking probability $S = 0.33$.

Fig. 11.— Column densities of assorted species for models with different initial conditions plotted vs R . The solid lines are the same as those of Figure 10. For the dotted lines, the initial central density is $n_{\text{H}} = 2.0 \times 10^2$ cm^{-3} . For the dashed lines, the gas has a pre-collapse phase of 3×10^5 yr in a cloud of constant density $n_{\text{H}} = 2.0 \times 10^4$ cm^{-3} . The physical structure of the three core models is the same, with the eventual central density $n_{\text{H}} = 3 \times 10^6$ cm^{-3} .

Fig. 12.— Column densities at $t = 1.89 \times 10^5$ yr plotted vs R for models with different adsorption energies: Model A (*solid lines*), Model B (*dotted lines*), and Model C (*dashed lines*). The Larson-Penston collapse ($f = 1$) is assumed. Descriptions of the models are given in §3.6.

Fig. 13.— The column density ratio of DCO^+ to HCO^+ plotted vs R . (a) The Larson-Penston core with $S = 1.0$ at $t = 1.52 \times 10^5$ yr (*dotted line*), 1.89×10^5 (*solid line*), and 2.00×10^5 (*dashed line*). (b) Thick lines for $t = f \times 1.89 \times 10^5$ yr; $f = 3$ for the dotted line, and $f = 10$ for the dashed line, while $f = 1$ for the solid line. Thin lines for $t = 1.89 \times 10^5$ yr with different sets of adsorption energies; the dotted line for Model B, and the dashed line for Model C (see §3.6).

TABLE 1
INITIAL ABUNDANCES ^a

Species	Abundance	Species	Abundance
H ₂	5.0(-1) ^b	HD	1.50(-5)
He	9.75(-2)	N	2.47(-5)
O	1.80(-4)	electrons	7.87(-5)
C ⁺	7.86(-5)	Na ⁺	2.25(-9)
Mg ⁺	1.09(-8)	Si ⁺	9.74(-9)
P ⁺	2.16(-10)	S ⁺	9.14(-8)
Cl ⁺	1.00(-9)	Fe ⁺	2.74(-9)
Grain	1.04(-2) ^c		

^aThe abundances by number of the species relative to hydrogen nuclei.

^b $a(b)$ means $a \times 10^b$.

^cThe abundance of refractory grain cores by mass relative to hydrogen.

TABLE 2
COLUMN DENSITY [cm⁻²] OF MOLECULES IN LARSON-PENSTON CORE AT $t = 1.89 \times 10^5$ YR AS A FUNCTION
OF DISTANCE FROM THE CENTER

Species	1000 AU	3000 AU	5000 AU	7000 AU	9000 AU	11000 AU	13000 AU
Gaseous Species							
C	2.29E+17	2.50E+17	2.77E+17	2.74E+17	2.53E+17	2.19E+17	1.66E+17
Cl	1.93E+13	2.07E+13	1.95E+13	1.61E+13	1.25E+13	9.16E+12	5.83E+12
Fe	7.84E+13	7.86E+13	6.67E+13	4.97E+13	3.41E+13	2.05E+13	9.25E+12
H	8.87E+19	9.11E+19	9.66E+19	1.08E+20	1.28E+20	1.58E+20	1.76E+20
D	1.25E+16	1.08E+16	1.02E+16	9.96E+15	9.53E+15	8.73E+15	7.08E+15
He	1.67E+22	8.32E+21	4.79E+21	3.08E+21	2.06E+21	1.36E+21	8.09E+20
Mg	1.86E+14	2.05E+14	2.01E+14	1.69E+14	1.30E+14	9.05E+13	5.10E+13
N	1.84E+18	1.37E+18	9.59E+17	6.68E+17	4.66E+17	3.17E+17	1.91E+17
Na	3.78E+13	4.16E+13	4.02E+13	3.34E+13	2.57E+13	1.86E+13	1.12E+13
O	8.39E+18	6.29E+18	4.48E+18	3.17E+18	2.26E+18	1.57E+18	9.77E+17
S	1.85E+15	1.93E+15	1.77E+15	1.43E+15	1.10E+15	7.88E+14	4.88E+14
Si	1.53E+14	1.69E+14	1.66E+14	1.38E+14	1.05E+14	7.25E+13	4.24E+13
C ₂	8.85E+13	9.28E+13	9.93E+13	1.07E+14	1.18E+14	1.32E+14	1.39E+14
CH	1.50E+13	1.58E+13	1.76E+13	1.92E+13	2.00E+13	1.96E+13	1.63E+13
CN	9.00E+14	9.96E+14	1.06E+15	9.83E+14	8.55E+14	6.98E+14	4.82E+14
CO	1.59E+18	1.70E+18	1.55E+18	1.21E+18	8.92E+17	6.11E+17	3.58E+17
CS	5.03E+13	5.48E+13	5.93E+13	5.84E+13	5.44E+13	4.90E+13	4.26E+13
H ₂	8.54E+22	4.26E+22	2.45E+22	1.57E+22	1.05E+22	6.91E+21	4.05E+21
HD	2.50E+18	1.25E+18	7.15E+17	4.57E+17	3.04E+17	2.00E+17	1.17E+17
N ₂	1.63E+16	1.08E+16	6.66E+15	4.11E+15	2.53E+15	1.45E+15	6.74E+14
NO	9.93E+14	5.36E+14	3.38E+14	2.36E+14	1.71E+14	1.21E+14	7.24E+13
O ₂	3.00E+16	3.37E+15	8.46E+14	4.41E+14	2.80E+14	1.85E+14	1.10E+14
OH	6.10E+13	3.96E+13	3.06E+13	2.56E+13	2.19E+13	1.83E+13	1.35E+13
SiO	1.94E+13	1.78E+13	1.59E+13	1.47E+13	1.43E+13	1.40E+13	1.05E+13
C ₂ H	1.93E+14	2.05E+14	2.31E+14	2.53E+14	2.58E+14	2.40E+14	1.77E+14
C ₂ N	6.21E+13	6.73E+13	7.53E+13	7.93E+13	7.49E+13	5.85E+13	2.95E+13
C ₂ S	2.54E+13	2.74E+13	3.17E+13	3.39E+13	3.11E+13	2.36E+13	1.24E+13
C ₃	5.24E+13	5.43E+13	5.84E+13	6.52E+13	7.46E+13	8.57E+13	9.15E+13
CH ₂	2.29E+15	2.53E+15	2.68E+15	2.46E+15	2.10E+15	1.67E+15	1.11E+15
CHD	9.63E+12	1.02E+13	1.02E+13	9.46E+12	8.32E+12	6.80E+12	4.25E+12
CO ₂	3.76E+15	3.47E+15	1.82E+15	5.77E+14	1.61E+14	4.64E+13	1.07E+13
H ₂ O	2.72E+16	2.26E+16	1.75E+16	1.18E+16	6.84E+15	3.10E+15	8.62E+14
HDO	9.57E+14	5.59E+14	3.57E+14	2.15E+14	1.12E+14	4.44E+13	1.01E+13
HCN	2.05E+15	2.34E+15	2.43E+15	1.93E+15	1.34E+15	7.76E+14	2.64E+14
DCN	1.58E+13	1.75E+13	1.68E+13	1.30E+13	9.05E+12	5.12E+12	1.59E+12
HNC	9.15E+14	1.05E+15	1.08E+15	8.28E+14	5.32E+14	2.58E+14	5.71E+13
DNC	2.00E+13	2.26E+13	2.09E+13	1.46E+13	8.92E+12	4.01E+12	6.45E+11
NH ₂	6.49E+12	6.00E+12	5.57E+12	4.91E+12	4.04E+12	2.90E+12	1.49E+12
OCN	6.43E+14	4.15E+14	2.40E+14	1.26E+14	5.65E+13	2.35E+13	7.91E+12
OCS	3.77E+13	4.44E+13	4.28E+13	2.76E+13	1.31E+13	4.69E+12	1.20E+12
C ₂ H ₂	2.94E+13	2.49E+13	2.15E+13	1.97E+13	1.79E+13	1.55E+13	1.17E+13
C ₃ H	2.44E+14	2.61E+14	2.93E+14	3.20E+14	3.23E+14	2.81E+14	1.66E+14
C ₃ N	4.71E+13	5.06E+13	5.72E+13	6.19E+13	6.06E+13	5.03E+13	2.82E+13
C ₄	3.30E+13	3.40E+13	3.65E+13	4.08E+13	4.70E+13	5.46E+13	6.08E+13
CH ₃	7.95E+12	8.40E+12	8.99E+12	9.43E+12	9.53E+12	9.06E+12	7.27E+12
H ₂ CO	4.32E+14	4.75E+14	5.13E+14	4.84E+14	3.85E+14	2.41E+14	9.73E+13
HDCO	1.76E+13	1.91E+13	1.98E+13	1.81E+13	1.43E+13	8.92E+12	3.56E+12
H ₂ CS	1.07E+13	1.24E+13	1.10E+13	7.12E+12	3.81E+12	1.64E+12	5.50E+11

TABLE 2—*Continued*

Species	1000 AU	3000 AU	5000 AU	7000 AU	9000 AU	11000 AU	13000 AU
NH ₃	3.31E+13	2.84E+13	2.27E+13	1.68E+13	1.15E+13	6.51E+12	2.44E+12
C ₂ H ₂ N	7.30E+14	8.57E+14	8.68E+14	6.24E+14	3.48E+14	1.35E+14	2.26E+13
C ₂ HDN	2.22E+13	2.52E+13	2.21E+13	1.43E+13	7.46E+12	2.77E+12	4.59E+11
C ₂ H ₂ O	2.60E+14	2.95E+14	3.31E+14	2.95E+14	1.98E+14	9.40E+13	2.59E+13
C ₂ H ₃	1.44E+14	1.57E+14	1.78E+14	1.89E+14	1.72E+14	1.22E+14	5.98E+13
C ₂ H ₂ D	8.38E+12	9.15E+12	1.03E+13	1.07E+13	9.58E+12	6.59E+12	2.97E+12
C ₃ H ₂	1.77E+13	1.87E+13	2.07E+13	2.33E+13	2.48E+13	2.36E+13	1.79E+13
C ₄ H	1.36E+14	1.44E+14	1.63E+14	1.87E+14	1.88E+14	1.56E+14	1.04E+14
C ₄ N	4.93E+12	5.29E+12	6.03E+12	6.58E+12	6.27E+12	4.91E+12	2.72E+12
C ₅	1.28E+13	1.32E+13	1.41E+13	1.59E+13	1.84E+13	2.12E+13	2.28E+13
CH ₂ O ₂	3.55E+13	3.60E+13	2.76E+13	1.58E+13	7.13E+12	2.19E+12	3.00E+11
CH ₄	4.01E+16	4.60E+16	4.54E+16	3.39E+16	2.08E+16	9.99E+15	3.00E+15
CH ₃ D	3.69E+15	4.22E+15	4.08E+15	3.02E+15	1.85E+15	8.82E+14	2.60E+14
HC ₃ N	1.62E+13	1.77E+13	2.05E+13	2.13E+13	1.86E+13	1.23E+13	4.43E+12
NH ₂ CN	9.35E+12	1.08E+13	1.16E+13	9.39E+12	6.23E+12	3.05E+12	7.98E+11
C ₂ H ₃ N	3.58E+13	3.94E+13	4.75E+13	4.82E+13	3.74E+13	1.89E+13	3.38E+12
C ₄ H ₂	2.55E+13	2.90E+13	3.15E+13	2.61E+13	1.46E+13	5.09E+12	1.00E+12
C ₅ H	5.85E+12	6.15E+12	6.84E+12	7.86E+12	8.63E+12	7.95E+12	4.71E+12
C ₅ N	4.92E+12	5.28E+12	5.99E+12	6.54E+12	6.29E+12	5.06E+12	3.01E+12
CH ₄ O	1.73E+13	1.98E+13	2.29E+13	1.98E+13	1.19E+13	4.43E+12	6.63E+11
C ₃ H ₄	2.02E+13	2.29E+13	2.76E+13	2.48E+13	1.44E+13	4.80E+12	7.04E+11
C ₅ H ₂	7.00E+12	7.58E+12	8.60E+12	9.32E+12	8.73E+12	6.16E+12	2.18E+12
HC ₅ N	1.64E+13	1.82E+13	2.13E+13	2.08E+13	1.51E+13	7.63E+12	2.02E+12
C ₆ H ₂	1.27E+13	1.38E+13	1.45E+13	1.35E+13	1.06E+13	6.81E+12	2.77E+12
CH ₃ C ₄ H	3.97E+13	4.55E+13	4.96E+13	4.11E+13	2.55E+13	1.09E+13	2.17E+12
e	4.19E+14	3.35E+14	2.78E+14	2.38E+14	2.06E+14	1.82E+14	1.64E+14
C ⁺	4.53E+13	4.30E+13	4.05E+13	4.04E+13	4.26E+13	4.84E+13	6.25E+13
Fe ⁺	1.16E+13	1.22E+13	1.26E+13	1.27E+13	1.29E+13	1.29E+13	1.15E+13
Mg ⁺	1.96E+13	2.09E+13	2.26E+13	2.34E+13	2.39E+13	2.43E+13	2.31E+13
Na ⁺	5.53E+12	6.06E+12	6.42E+12	6.09E+12	5.38E+12	4.54E+12	3.76E+12
C ₂ N ⁺	4.53E+12	5.10E+12	5.27E+12	4.61E+12	3.91E+12	3.15E+12	1.85E+12
H ₃ ⁺	1.65E+13	1.18E+13	9.29E+12	7.81E+12	6.60E+12	5.34E+12	3.73E+12
HCO ⁺	6.88E+13	6.52E+13	5.41E+13	4.30E+13	3.33E+13	2.35E+13	1.23E+13
H ₂ CN ⁺	1.68E+13	1.93E+13	1.90E+13	1.39E+13	8.74E+12	4.30E+12	1.05E+12
H ₃ O ⁺	1.59E+14	9.50E+13	6.16E+13	4.25E+13	2.90E+13	1.80E+13	8.09E+12
Mantle Species							
C	7.60E+16	7.05E+16	5.36E+16	3.62E+16	2.43E+16	1.63E+16	9.93E+15
Cl	1.44E+14	5.97E+13	2.77E+13	1.45E+13	8.14E+12	4.63E+12	2.41E+12
Fe	3.71E+14	1.35E+14	5.31E+13	2.29E+13	1.00E+13	4.07E+12	1.32E+12
Mg	1.64E+15	6.79E+14	3.04E+14	1.48E+14	7.42E+13	3.58E+13	1.46E+13
N	2.10E+18	6.07E+17	2.07E+17	8.75E+16	4.23E+16	2.16E+16	1.04E+16
Na	3.36E+14	1.39E+14	6.24E+13	3.10E+13	1.61E+13	8.19E+12	3.48E+12
O	9.26E+18	2.70E+18	9.41E+17	4.08E+17	2.02E+17	1.06E+17	5.29E+16
P	2.85E+13	1.21E+13	5.71E+12	3.02E+12	1.70E+12	9.53E+11	4.73E+11
S	1.17E+16	4.81E+15	2.19E+15	1.12E+15	6.15E+14	3.36E+14	1.62E+14
Si	1.36E+15	5.62E+14	2.52E+14	1.23E+14	6.33E+13	3.23E+13	1.46E+13
C ₂	4.27E+15	2.29E+15	1.43E+15	9.86E+14	7.08E+14	4.99E+14	3.12E+14
CN	1.25E+16	5.64E+15	2.87E+15	1.63E+15	9.71E+14	5.67E+14	2.91E+14
CO	1.06E+19	4.12E+18	1.75E+18	8.33E+17	4.25E+17	2.18E+17	1.02E+17

TABLE 2—*Continued*

Species	1000 AU	3000 AU	5000 AU	7000 AU	9000 AU	11000 AU	13000 AU
CS	9.53E+14	4.06E+14	2.03E+14	1.18E+14	7.63E+13	5.25E+13	3.46E+13
N ₂	5.70E+16	1.46E+16	4.67E+15	1.87E+15	8.22E+14	3.49E+14	1.23E+14
NO	3.27E+15	8.99E+14	3.50E+14	1.76E+14	9.63E+13	5.09E+13	2.21E+13
O ₂	4.39E+16	2.92E+15	6.12E+14	2.71E+14	1.44E+14	7.78E+13	3.63E+13
OH	3.95E+14	1.56E+14	7.99E+13	4.83E+13	3.06E+13	1.87E+13	9.71E+12
SiO	9.70E+13	4.53E+13	2.57E+13	1.64E+13	1.05E+13	5.95E+12	2.42E+12
SO	3.07E+13	8.13E+12	1.88E+12	3.88E+11	8.35E+10	1.91E+10	3.66E+09
C ₂ H	5.47E+15	2.46E+15	1.26E+15	7.05E+14	4.02E+14	2.16E+14	9.44E+13
C ₂ N	1.14E+15	4.99E+14	2.35E+14	1.16E+14	5.45E+13	2.23E+13	6.46E+12
C ₂ S	3.36E+14	1.40E+14	6.54E+13	3.28E+13	1.61E+13	7.10E+12	2.46E+12
C ₃	1.93E+15	1.06E+15	6.63E+14	4.58E+14	3.28E+14	2.29E+14	1.41E+14
CH ₂	1.44E+16	6.99E+15	3.60E+15	2.00E+15	1.17E+15	6.73E+14	3.33E+14
CHD	4.52E+13	2.28E+13	1.25E+13	7.47E+12	4.53E+12	2.53E+12	1.05E+12
CO ₂	3.22E+16	6.92E+15	1.22E+15	2.10E+14	4.17E+13	8.88E+12	1.50E+12
H ₂ O	2.55E+17	8.22E+16	2.82E+16	1.02E+16	3.51E+15	1.02E+15	2.09E+14
HDO	5.62E+15	1.52E+15	4.63E+14	1.52E+14	4.68E+13	1.17E+13	1.90E+12
HCN	2.71E+16	9.82E+15	3.78E+15	1.55E+15	6.21E+14	2.11E+14	4.58E+13
DCN	1.60E+14	5.92E+13	2.34E+13	9.89E+12	4.04E+12	1.34E+12	2.75E+11
HCO	1.09E+14	3.19E+13	8.29E+12	1.87E+12	4.22E+11	1.13E+11	3.22E+10
HNC	1.21E+16	4.31E+15	1.58E+15	5.99E+14	2.11E+14	5.67E+13	8.25E+12
DNC	2.01E+14	6.85E+13	2.39E+13	8.66E+12	2.93E+12	7.03E+11	6.77E+10
HNO	5.49E+13	1.92E+13	7.45E+12	3.10E+12	1.26E+12	4.57E+11	1.27E+11
N ₂ O	7.35E+13	1.95E+13	5.38E+12	1.61E+12	4.85E+11	1.33E+11	2.91E+10
OCN	2.39E+15	6.34E+14	1.88E+14	5.92E+13	1.86E+13	5.68E+12	1.35E+12
OCS	3.17E+14	1.03E+14	3.23E+13	9.72E+12	2.70E+12	6.69E+11	1.30E+11
C ₂ H ₂	2.08E+14	9.40E+13	5.17E+13	3.25E+13	2.11E+13	1.33E+13	7.31E+12
C ₃ H	5.16E+15	2.33E+15	1.17E+15	6.15E+14	3.13E+14	1.39E+14	4.48E+13
C ₃ D	5.88E+13	2.66E+13	1.31E+13	6.76E+12	3.27E+12	1.31E+12	3.28E+11
C ₃ N	7.71E+14	3.40E+14	1.65E+14	8.42E+13	4.17E+13	1.82E+13	5.77E+12
C ₃ S	4.03E+13	1.59E+13	7.22E+12	3.66E+12	1.90E+12	9.62E+11	4.24E+11
C ₄	9.71E+14	5.32E+14	3.35E+14	2.34E+14	1.71E+14	1.24E+14	7.97E+13
CH ₃	1.33E+14	7.14E+13	4.37E+13	2.92E+13	1.99E+13	1.31E+13	7.42E+12
H ₂ CO	6.20E+15	2.56E+15	1.13E+15	5.17E+14	2.25E+14	8.41E+13	2.35E+13
HDCO	2.04E+14	8.47E+13	3.80E+13	1.77E+13	7.85E+12	2.97E+12	8.14E+11
H ₂ CS	5.15E+13	1.88E+13	6.77E+12	2.49E+12	8.81E+11	2.83E+11	7.36E+10
NH ₃	3.09E+14	1.13E+14	4.62E+13	2.07E+13	9.03E+12	3.39E+12	9.33E+11
C ₂ H ₂ N	8.63E+15	2.95E+15	1.01E+15	3.41E+14	1.00E+14	2.11E+13	2.07E+12
C ₂ HDN	1.91E+14	6.21E+13	2.02E+13	6.55E+12	1.89E+12	3.98E+11	3.87E+10
C ₂ H ₂ O	3.16E+15	1.22E+15	4.87E+14	1.92E+14	6.71E+13	1.87E+13	3.25E+12
C ₂ HDO	1.00E+14	3.87E+13	1.54E+13	6.06E+12	2.10E+12	5.66E+11	8.75E+10
C ₂ H ₃	2.37E+15	1.07E+15	5.29E+14	2.70E+14	1.30E+14	5.45E+13	1.71E+13
C ₂ H ₂ D	1.20E+14	5.41E+13	2.65E+13	1.34E+13	6.33E+12	2.49E+12	6.79E+11
C ₃ H ₂	3.88E+14	1.89E+14	1.02E+14	5.90E+13	3.45E+13	1.92E+13	9.05E+12
C ₄ H	4.22E+15	1.74E+15	7.88E+14	3.91E+14	2.00E+14	9.98E+13	4.35E+13
C ₄ N	1.05E+14	4.56E+13	2.11E+13	1.01E+13	4.58E+12	1.86E+12	5.84E+11
C ₅	5.44E+14	2.83E+14	1.68E+14	1.11E+14	7.71E+13	5.37E+13	3.45E+13
CH ₂ O ₂	2.04E+14	6.44E+13	1.97E+13	5.87E+12	1.52E+12	2.81E+11	2.46E+10
CH ₄	4.24E+17	1.72E+17	6.99E+16	2.82E+16	1.05E+16	3.23E+15	6.55E+14
CH ₃ D	3.65E+16	1.47E+16	5.93E+15	2.39E+15	8.92E+14	2.71E+14	5.32E+13

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TABLE 2—*Continued*

Species	1000 AU	3000 AU	5000 AU	7000 AU	9000 AU	11000 AU	13000 AU
HC ₃ N	2.55E+14	1.05E+14	4.64E+13	2.10E+13	8.77E+12	2.94E+12	6.06E+11
NH ₂ CN	1.49E+14	5.59E+13	2.19E+13	8.67E+12	3.10E+12	8.46E+11	1.38E+11
C ₂ H ₃ N	8.04E+14	2.88E+14	1.11E+14	4.30E+13	1.46E+13	3.39E+12	3.23E+11
C ₃ H ₃	4.80E+13	2.18E+13	1.01E+13	4.38E+12	1.60E+12	4.01E+11	4.59E+10
C ₄ H ₂	2.46E+14	1.03E+14	4.14E+13	1.47E+13	4.20E+12	9.00E+11	1.33E+11
C ₅ H	2.51E+14	1.07E+14	4.90E+13	2.35E+13	1.08E+13	4.38E+12	1.38E+12
C ₅ N	9.66E+13	4.25E+13	2.00E+13	9.78E+12	4.63E+12	1.99E+12	6.81E+11
C ₆	2.29E+14	1.13E+14	6.31E+13	3.83E+13	2.39E+13	1.48E+13	8.49E+12
CH ₄ O	3.57E+14	1.30E+14	4.68E+13	1.58E+13	4.45E+12	8.66E+11	7.99E+10
C ₃ H ₄	2.70E+14	1.12E+14	4.48E+13	1.57E+13	4.29E+12	7.82E+11	7.21E+10
C ₃ H ₃ D	1.96E+13	8.14E+12	3.24E+12	1.13E+12	3.05E+11	5.38E+10	4.53E+09
C ₅ H ₂	1.28E+14	5.84E+13	2.78E+13	1.30E+13	5.31E+12	1.64E+12	2.68E+11
C ₆ H	1.89E+14	7.47E+13	3.16E+13	1.37E+13	5.55E+12	1.85E+12	4.22E+11
C ₇	1.00E+14	4.83E+13	2.59E+13	1.50E+13	8.78E+12	5.00E+12	2.66E+12
HC ₅ N	2.79E+14	1.06E+14	4.10E+13	1.54E+13	5.10E+12	1.31E+12	2.00E+11
C ₆ H ₂	1.35E+14	6.01E+13	2.76E+13	1.26E+13	5.25E+12	1.77E+12	3.63E+11
C ₇ H	1.21E+14	4.43E+13	1.71E+13	6.76E+12	2.46E+12	7.05E+11	1.05E+11
C ₈	4.59E+13	2.10E+13	1.04E+13	5.43E+12	2.77E+12	1.30E+12	5.38E+11
C ₇ H ₂	5.20E+13	2.05E+13	8.21E+12	3.15E+12	1.05E+12	2.65E+11	4.12E+10
C ₈ H	1.08E+14	4.02E+13	1.58E+13	6.36E+12	2.38E+12	7.34E+11	1.42E+11
CH ₃ C ₄ H	3.60E+14	1.49E+14	6.09E+13	2.33E+13	7.44E+12	1.68E+12	1.79E+11
HC ₇ N	5.05E+13	1.86E+13	7.06E+12	2.62E+12	8.48E+11	1.97E+11	1.97E+10
C ₈ H ₂	6.27E+13	2.54E+13	1.04E+13	4.05E+12	1.35E+12	3.23E+11	3.76E+10
C ₉ H ₂	3.04E+13	1.04E+13	3.51E+12	1.12E+12	2.92E+11	5.20E+10	3.68E+09
HC ₉ N	2.16E+13	7.39E+12	2.55E+12	8.33E+11	2.27E+11	4.19E+10	3.07E+09

TABLE 3
ADSORPTION ENERGIES (K)

Species	Model A ^a	Model B ^b
CO	1210	960
N ₂	1210	750
CO ₂	2500	2690
H ₂ O	1860	4820
HCN	1760	4280
SO ₂	3070	3460
C ₂ H ₂	1610	2490
NH ₃	1110	3080
CH ₄	1360	1120

^aHasegawa & Herbst 1993^bSee text for references.

TABLE 4
MOLECULAR COLUMN DENSITIES IN COLLAPSING CORE

	CCS	CO	N ₂ H ⁺
L1544	$N_{\text{peak}} = 4 \times 10^{13} \text{ cm}^{-2}$ ^a $R_{\text{hole}} \sim 7500 \text{ AU}$ ^a	$N_{\text{peak}} = 2 \times 10^{18} \text{ cm}^{-2}$ ^b $R_{\text{hole}} \sim 6500 \text{ AU}$ ^d	$N_{\text{peak}} = 6 \times 10^{12} \text{ cm}^{-2}$ ^c centrally peaked
f=1,S=1.0	$N_{\text{peak}} = 3.3 \times 10^{13} \text{ cm}^{-2}$ $R_{\text{hole}} \sim 7000 \text{ AU}$	$N_{\text{peak}} = 1.7 \times 10^{18} \text{ cm}^{-2}$ $R_{\text{hole}} \sim 4000 \text{ AU}$	$N_{\text{peak}} = 2.5 \times 10^{11} \text{ cm}^{-2}$ centrally peaked
f=3,S=1.0	$N_{\text{peak}} = 1.4 \times 10^{12} \text{ cm}^{-2}$ $R_{\text{hole}} = 13000 \text{ AU}$	$N_{\text{peak}} = 4.7 \times 10^{17} \text{ cm}^{-2}$ $R_{\text{hole}} = 7500 \text{ AU}$	$N_{\text{peak}} = 1.4 \times 10^{12} \text{ cm}^{-2}$ centrally peaked
f=10,S=1.0	$N_{\text{peak}} = 8.0 \times 10^9 \text{ cm}^{-2}$ $R_{\text{hole}} = 14000 \text{ AU}$	$N_{\text{peak}} = 9.5 \times 10^{16} \text{ cm}^{-2}$ centrally peaked	$N_{\text{peak}} = 2.4 \times 10^{12} \text{ cm}^{-2}$ centrally peaked
f=3,S=0.3	$N_{\text{peak}} = 4.3 \times 10^{12} \text{ cm}^{-2}$ $R_{\text{hole}} = 12000 \text{ AU}$	$N_{\text{peak}} = 1.7 \times 10^{18} \text{ cm}^{-2}$ $R_{\text{hole}} = 4000 \text{ AU}$	$N_{\text{peak}} = 9.9 \times 10^{11} \text{ cm}^{-2}$ centrally peaked

^aOhashi et al. 1999

^bCaselli 2000, private communication

^cBenson et al. 1998

^dCaselli et al. 1999

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